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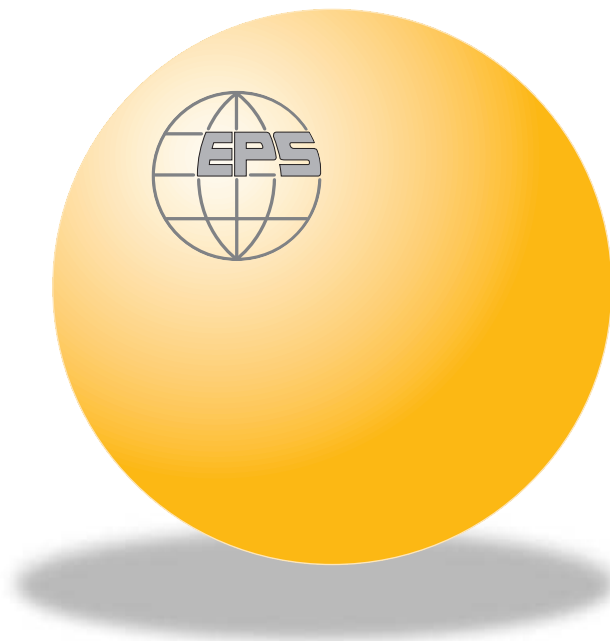
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Compression modulus of macroscopic fiber bundles

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Abstract. – We study dense, disordered stacks of elastic macroscopic fibers. These stacks often exhibit non-linear elasticity, due to the coupling between the applied stress and the internal distribution of fiber contacts. We propose a theoretical model for the compression modulus of such systems, and illustrate our method by studying the conical shapes frequently observed at the extremities of ropes and other fiber structures.

Threadlike objects are the constituents of many natural and synthetic materials [1,2]. At the microscopic level, filaments such as actin, microtubules and other semi-flexible polymers control not only the elastic and viscous properties of different biological architectures [3] but also of polymer melts, surfactant solutions and gels [4]. These are collective properties that can be understood from the individual characteristics of the filaments like the bending and stretching elasticity or the friction coefficient [5]. At such small scales, thermal disorder plays a key role that has been successfully described within the framework of statistical mechanics. For instance, the reptation theory for polymer melts and solutions [4,6] or the description of rigid gel elasticity [7] successfully account for the collective macroscopic behavior, based on a few, microscopic parameters of the single polymers. Surprisingly, macroscopic threadlike systems have been much less studied, in spite of their abundance in the natural and synthetic realms: hair, wool, cotton and other natural fibers or Nylon strings, ropes and textiles or glass wool belong to this class of systems [2]. Here also the elastic or friction constitutive parameters of the individual objects are well known. For instance, bending and stretching moduli of human hair, wool, Nylon and steel fibers can easily be found in the literature. But theories that predict collective fiber properties such as the compressibility of a hair tress, or studies that explain what forces play a role in a disentanglement action like combing or carding, are scarce [8,9]. In this letter we argue that methods developed for fiber microscopic systems [10] are also useful at the macroscopic level, and draw an analogy between the effect of thermal fluctuations and the effect of the intrinsic disorder carried by the spontaneous shapes of the fibers.
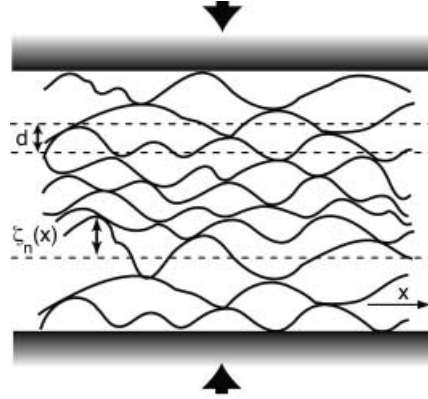
Fig. 1 – Dense fiber bundle. The function $\zeta_n(x)$ describes the shape of the n-th fiber with respect to a reference average level.

We consider a two-dimensional fiber bundle as illustrated in fig. 1. Discussion in two dimensions allows for a simpler presentation of the methods, while retaining the main ingredients of the problem. Extension to the three-dimensional case will be discussed later. The bundle is composed of a large number $\mathcal{N}$ of elastic strands of length L, in a space of height $d \times \mathcal{N}$, where d is the average distance between two fibers. The shape of the fiber is described by the function $\zeta_n(x)$ that measures height deviations from the line of average position at height $d \times n$. This description in the Monge parametrization is well adapted to the shapes of interest, with a weak gradient $\mathrm{d}\zeta_n(x)/\mathrm{d}x \ll 1$. In the absence of interactions between fibers, each filament n has a spontaneous shape, described by the function $\zeta_{0,n}(x)$. It is the disorder associated with the spontaneous shapes of the different fibers that leads to a non-trivial compression behavior of the whole system. Under an external force, the spontaneous shape of the fiber $\zeta_{0,n}(x)$ will be transformed into the actual shape $\zeta_n(x)$. Within the elastic limit, the deformation of a segment of length $\mathrm{d}x$ around the natural shape will cost an elastic energy $\mathrm{d}U_{\mathrm{b}}$, proportional to the bending modulus κ and to the curvature differences, $\mathrm{d}U_{\mathrm{b}} = \kappa/2(\zeta_n''(x) - \zeta_{0,n}''(x))^2\,\mathrm{d}x$. The bending modulus κ is a constitutive property of the fiber, that depends on the shape of its section and on the Young modulus of the material [5]. For instance, for a cylindral filament of radius a and Young modulus E one has $\kappa = Ea^4/4$. The total bending energy of the $\mathcal{N}$ filaments can then be written as

$$U_{\mathrm{b}} = \frac{\kappa}{2} \sum_{n=1}^{\mathcal{N}} \int_0^L \mathrm{d}x \left[\zeta_n''(x) - \zeta_{0,n}''(x) \right]^2. \tag{1}$$

If one assumes that different fibers interact through a two-body potential V, then the total interaction energy U_{int} can be written as

$$U_{\mathrm{int}} = \sum_{n,m=1}^{\mathcal{N}} \int_0^L \mathrm{d}x \int_0^L \mathrm{d}x' V \left[\zeta_m(x) + md - \left(\zeta_n(x') + nd \right) \right]. \tag{2}$$

In order to bring the structure of the interaction energy to a tractable level, we follow a simple mean-field approximation, similar to the Helfrich treatment of thermally activated fluid membranes and fibers [11, 12]. We assume that forces between first neighbors dominate the interaction energy, an exact assumption for excluded-volume potentials and a good approximation for other short-range forces such as those given by screened electrostatic potentials. Then

the sum of the bending (1) and interaction (2) terms can be written as the effective energy:

$$E_{\text{eff}} = \frac{\kappa}{2} \sum_{n=1}^{\mathcal{N}} \int_0^L \mathrm{d}x \left[\zeta_n''(x) - \zeta_{0,n}''(x) \right]^2 + \frac{B}{2} \sum_{n=1}^{\mathcal{N}} \int_0^L \mathrm{d}x \left[\zeta_{n+1}(x) - \zeta_n(x) \right]^2. \tag{3}$$

Because of the weak gradients involved, inter-fiber interactions take place only at the same x coordinate. B is the strength of the mean-field quadratic potential, to be determined by the self-consistent prescription $B = d \times \partial^2 \langle e \rangle / \partial d^2$, where $\langle e \rangle = \langle E_{\text{eff}} \rangle / (L\mathcal{N}d)$ is the average energy density. The equilibrium state of the fiber stack corresponds to the minimum of the effective energy functional (3) with respect to the fiber configurations $\{\zeta_n(x)\}$, given the spontaneous shapes $\{\zeta_{0,n}(x)\}$, or more precisely, given the spontaneous curvatures $\{\zeta_{0,n}''(x)\}$. The spontaneous curvatures are to be treated as the random functions responsible for disorder in the system. Averages, denoted by $\langle \rangle$, will then be performed with the probability associated with the spontaneous curvature distribution. Before carrying forward the outlined procedure, it is of interest to review results for the thermal case, as this will help to build intuition for the key quantities controlling the stack structure.

In thermal stacks or bundles of fibers, disorder is introduced by the random Brownian motion of the fibers, which would otherwise be flat, *i.e.* $\{\zeta_{0,n}(x) = 0\}$. The shape of a single fiber in solution is described by a persistent walk, a class of statistical walks where tangent correlations vanish exponentially over a persistence length ℓ_{p}, related to the fiber rigidity through $\ell_{\text{p}} = \kappa / (k_{\text{B}}T)$. A persistent walk primarily moves along the forward direction for a short enough distance ℓ, but it also performs side excursions of size D. From the equipartition theorem one has $\ell_{\text{p}} D^2 / \ell^3 \simeq 1$. In a stack, lateral excursions are limited by near neighbors setting $D = d$. Typically, there is one interaction between fibers over a collision distance $\ell_{\text{c}} \simeq \ell_{\text{p}}^{1/3} d^{2/3}$. Since the energy density of the thermal stack $\langle e_{\text{T}} \rangle$, is of the order of $k_{\text{B}}T$ per collision area, $\langle e_{\text{T}} \rangle \simeq k_{\text{B}}T / (d\ell_{\text{c}})$, one gets a compression modulus

$$B_{\text{T}} \simeq \frac{k_{\text{B}}T}{d^3} \left(\frac{d}{\ell_{\text{p}}} \right)^{1/3} = (k_{\text{B}}T)^{4/3} \kappa^{-1/3} d^{-8/3}, \tag{4}$$

which holds for large enough rigidities, $\ell_{\text{p}} \gg d$.

In macroscopic fiber stacks, the disorder is quenched and introduced by the spontaneous disordered shapes $\zeta_{0,n}(x)$. Let us consider a typical shape of amplitude ζ_0 and wavelength q_0^{-1}. Clearly, there are no interactions for distances larger than the shape amplitude, $d \gg \zeta_0$. For smaller distances, the local gradients are of order of $\zeta_0 q_0$, leading to a collision length $\ell_{\text{c}} \simeq d / (\zeta_0 q_0)$. The energy density is thus given by $\langle e \rangle \simeq \kappa \zeta_0^2 q_0^4 \ell_{\text{c}} / (d\ell_{\text{c}}) = \kappa \zeta_0^2 q_0^4 / d$, independent of ℓ_{c}. It follows that the compression modulus reads

$$B \simeq \kappa q_0^4 \left(\frac{\zeta_0}{d} \right)^2. \tag{5}$$

It is worthy at this stage to stress several striking differences and similarities between the thermal and the macroscopic cases. First, contrary to thermal stacks, where the compressibility is only governed by the persistence length ℓ_{p} and by the distance between fibers d, in macroscopic fiber stacks the spatial scale associated with disorder inhomogeneities also plays an important role. As a matter of fact, the scale for compressibility is set by the combination κq_0^4: stiffer fibers lead to harder macroscopic materials, quite opposite to thermal stacks where increasing fiber stiffness reduces fluctuations and softens the stack. Also, while the cost of confinement for thermally controlled fluctuations diverges as the confinement distance

vanishes, only a finite amount of energy is required to completely flatten a macroscopic fiber. But in both cases, the compression moduli increase with the degree of disorder, measured by the temperature in the thermal system, and by the square amplitude of spontaneous shapes, ζ_0^2 for the quenched bundle. And finally, the power law dependence of the thermal modulus is larger than the macroscopic one: quenched disorder appears to lead to more "robust" materials as these are less susceptible to variations in stack density. We now return to a more detailed calculation of the compression modulus.

It is convenient to perform the functional minimization of the effective energy (3) in the space of the eigenfunctions $\{\Phi_q\}$ for the biharmonic operator, $(\partial^4/\partial x^4 - q^4)\Phi_q(x) = 0$. We also choose boundary conditions ensuring that there are no forces nor torques on the strands extremities: $\Phi_q^{(2)}(0) = \Phi_q^{(2)}(L) = 0$ and $\Phi_q^{(3)}(0) = \Phi_q^{(3)}(L) = 0$. The orthonormal set of eigenfunctions can be written as

$$\phi_q(x) = \frac{\cosh(\alpha_{\mathrm{p}}) - \cos(\alpha_{\mathrm{p}})}{\sinh(\alpha_{\mathrm{p}}) - \sin(\alpha_{\mathrm{p}})} \left[\sinh\left(\alpha_{\mathrm{p}}\frac{x}{L}\right) + \sin\left(\alpha_{\mathrm{p}}\frac{x}{L}\right) \right] - \left[\cosh\left(\alpha_{\mathrm{p}}\frac{x}{L}\right) + \cos\left(\alpha_{\mathrm{p}}\frac{x}{L}\right) \right], \quad (6)$$

where the numerical coefficients α_{p} are determined from the relation $\cos(\alpha_{\mathrm{p}})\cosh(\alpha_{\mathrm{p}}) = 1$. The solutions obey approximately $\alpha_{\mathrm{p}} \equiv qL \simeq (p + \frac{1}{2})\pi$ with $p \in \mathbb{N}$. We first develop the shapes $\zeta_n(x)$ and $\zeta_{0,n}(x)$ on the basis of the eigenfunctions (6),

$$\zeta_n(x) = \frac{1}{\sqrt{\mathcal{N}L}} \sum_{q=\frac{\pi}{2L}}^{+\infty} \sum_{Q=-\frac{\pi}{d}}^{\frac{\pi}{d}} \zeta_{qQ}\phi_q(x)e^{iQnd}, \quad (7)$$

$$\zeta_{0,n}(x) = \frac{1}{\sqrt{\mathcal{N}L}} \sum_{q=\frac{\pi}{2L}}^{+\infty} \sum_{Q=-\frac{\pi}{d}}^{\frac{\pi}{d}} \zeta_{0,qQ}\phi_q(x)e^{iQnd}, \quad (8)$$

where Q is a wave vector along the stack direction, then minimise with respect to the coefficients ζ_{qQ} and finally compute the average energy density:

$$\langle e \rangle = \frac{1}{2L\mathcal{N}d} \sum_{q,Q} \frac{q^4 \langle \zeta_{0,qQ}{}^2 \rangle B(Q)}{q^4 + \frac{B(Q)}{\kappa}}, \quad (9)$$

where $B(Q) = 2B(1 - \cos Qd)$. Equation (9) shows how the spatial inhomogeneities of spontaneous shapes determine the energy density of the stack: the harmonic, elastic nature of the energy penalty for shape distortion and interfiber interactions translates into the sole dependence of the energy density on the values of the second moment of the shape disorder distribution, weighted by the classical correlation kernel for bending elasticity. A practical consequence of eq. (9) is that it allows to connect fiber geometric information, available from a simple statistical analysis on fiber shapes, with collective properties such as the compression modulus B. As an example, we now calculate the compression modulus for monomodal structures of uncorrelated fibers, for which the standard square deviation is written as $\langle \zeta_{0,qQ}{}^2 \rangle = \mathcal{N}L\zeta_0^2\delta_{qq_0}$. In the limit where $\mathcal{N} \gg 1$, the dimensionless compression modulus $\widetilde{B} = B/(\kappa q_0^4)$ obeys the self-consistent differential equation

$$\widetilde{B} = \widetilde{d}\frac{\partial^2}{\partial\widetilde{d}^2}\frac{1}{2\widetilde{d}}\left[1 - \left(1 + 4\widetilde{B}\right)^{-1/2}\right], \quad (10)$$

where ζ_0 now sets the natural distance units, $\widetilde{d} = d/\zeta_0$. At short distances, the compression modulus is high, and eq. (10) leads to the asymptotic form discussed in (5), $B = \kappa q_0^4\zeta_0^2/d^2$.
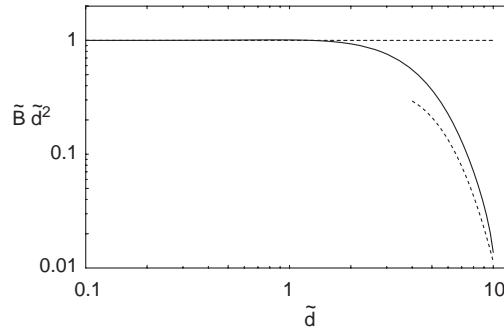
Fig. 2 – The full line is the compression modulus B of a fiber stack *vs.* interfiber distance d. Dashed lines represent the asymptotic behaviours at short distances, $\widetilde{B}\widetilde{d}^2 \simeq 1$, for $\widetilde{d} \ll 1$ and at large distances $\widetilde{B} \sim \widetilde{d}\exp[-\widetilde{d}]$, for $\widetilde{d} \gg 1$. Plots are for dimensionless quantities $\widetilde{B} = B/(\kappa q_0^4)$ and $\widetilde{d} = d/\zeta_0$, with κ the fiber rigidity, q_0 and ζ_0 the typical wave vector and amplitude of spontaneous shape disorder.

For distances larger than the natural amplitude for spontaneous shape disorder, ζ_0, the fibers do not interact significantly, and the compression modulus vanishes exponentially: $B = \kappa q_0^4 (d/\zeta_0) \exp[-d/\zeta_0]$. A numerical solution of eq. (10) interpolating between these two regimes is presented in fig. 2.

We now illustrate our results by studying the shape of the cones that appear at the end of ropes and other fiber bundles. The cones are generated by the expansion of the fibers, under the repulsive field that we discussed previously. The repulsive field experienced by one fiber, $U(d) = B(d)d^2/2$, can be roughly approximated by a step function of amplitude $\kappa q_0^4 \zeta_0^2/2$ and range ζ_0. The average path of one fiber is a straight, horizontal line, as long as it remains inside the constrained zone, as depicted in fig. 3. When it escapes confinement, the fiber crosses an expanding zone where it still interacts with its neighbors. Under the repulsive forces, the fiber bends until it escapes the repulsive potential, for interfiber distances larger than the range of the potential ζ_0. Bending of the fiber is caused by two localized forces of amplitude $f = \kappa q_0^4 \zeta_0^2/2$ and opposite signs, applied by the two closest neighbors. After escaping the expanding interaction zone, the fiber follows a straight line, at an angle that depends on its distance from the center of the bundle. If one enumerates the fibers in the stack from $n = 1$ in the center to $n = \mathcal{N}/2$ for the external fiber, the following set of equations
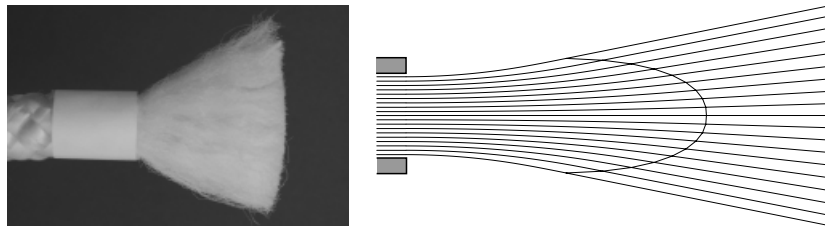

Fig. 3 – Cones are formed at the unconstrained ends of ropes and other bundles of fibers, as shown on the left for a Nylon rope. On the right, the calculated shape in two dimensions. Here, only the average fiber path is represented for simplicity. The fibers only interact mutually in the expansion zone, to the left of the curved line, and follow a straight path otherwise. The size of the expansion zone and the angle of the cone are independent of fiber rigidity, they are fully determined by the geometric properties of fiber disorder.
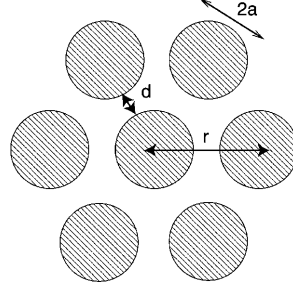
Fig. 4 – Cross-section of a three-dimensional bundle in the high-density limit where each fiber is confined in a cage defined by its first nearest neighbors.

recursively determine the position $[\ell_n, y_n]$ where a fiber escapes its neighbors potential:

$$(\ell_{n-1} - \ell_n)\big(3\ell_{n-1}^2 - (\ell_{n-1} - \ell_n)^2\big) \;=\; \frac{6\kappa}{f}\big(y_{n-1} - (n-1)d\big), \qquad (11)$$

$$(\ell_{n-1} - \ell_n)\ell_n^2 \;=\; \frac{2\kappa}{f}\big(y_n - nd - (\zeta_0 - d)\big), \qquad (12)$$

where ℓ_n is measured from the border of the confinement zone and y_n from the center of the stack. The distance d is the interfiber separation in the confinement zone. Equations (12) and the boundary conditions $y_1 = \zeta_0$ and $\ell_{\mathcal{N}/2}^3 = (y_{\mathcal{N}/2} - d\mathcal{N}/2)3\kappa/f$ determine the shape to the boundary $y_n(\ell_n)$, also shown in fig. 3. The extension of the expansion zone, ℓ_1, depends on the number of fibers and on the compression rate $\alpha = (\zeta_0 - d)/\zeta_0$, but not on the fiber rigidity: $\ell_1 \sim \zeta_0 \mathcal{N}^{2/3} \alpha^{1/3} (q_0\zeta_0)^{-4/3}$. Similarly, the geometric shape of the cone, given by the slope of the last fiber $\theta_{\mathcal{N}/2}$, does not depend on the fiber rigidity, it is only fixed by the geometric quantities associated with the fiber disorder, $\theta_{\mathcal{N}/2} \sim \alpha^{2/3}(q_0\zeta_0)^{-4/3}$.

For high enough fiber density, the compression modulus of a three-dimensional bundle can be computed in a manner similar to the two-dimensional case. Indeed, if the density is so high as to provide a cage environment for each of the fibers, as depicted in fig. 4, the forces between fibers are controlled by excluded-volume interactions between near-neighbors. In this case, we define a two-dimensional fiber density in the bundle $\sigma = \mathcal{N}\pi a^2/\mathcal{A}$, where $\mathcal{A}$ is the area of the bundle section. For a perfectly ordered hexagonal array, one would have $\sigma = 2\pi\sqrt{3}/3a^2 r^{-2}$, where r is the distance between fiber centers. The maximum close-packing density is $\sigma_{\max} \simeq 0.91$. The relevant fluctuating distance $d = r - 2a$ is now a function of the fiber density σ. In the hexagonal case, the cage would hold up to distances $d = 2a$ or densities as small as $\sigma_c = \pi\sqrt{3}/24 \simeq 0.23$. In this regime, the compression modulus is expected to vary as $B_{3D} \sim \kappa q_0^4 \zeta_0^2 r^{-3}$. As explained above, for the non-thermal case, only a finite energy is required to completely flatten a fiber. Thus, the confinement energy density is here bound to a maximum value $\langle e_{3D} \rangle \sim \kappa q_0^4 \zeta_0^2 a^{-2}$, contrary to the three-dimensional thermal situation [10], where the energy density diverges as $\sim d^{8/3}$. For densities smaller than σ_c, the situation is unclear, even for the thermal case. Large lateral excursions of the fiber are now possible [13], and there is not yet, to our knowledge, a clear criterium to determine the maximum allowed size of the excursions. We hope to address this question in future work.

As a summary, we have shown that stacks of macroscopic disordered fibers behave as a compressible material, the compression modulus being *proportional* to fiber rigidity, opposite to microscopic fiber stacks where it *decreases* with fiber rigidity. We have also shown how the compression modulus depends on stack density and on the geometric quantities characterizing

spontaneous shape disorder. Our results allow to predict collective properties from the individual fiber characteristics and provide a new tool to interpret experiments in fiber systems. As an example of this, we studied terminal bundle cones, showing that this class of shapes follows a universal behavior that depends only on the fiber geometric features. Extension of our results to three dimensions is straightforward in the limit of large fiber density. The weak-density limit poses an interesting challenge for fiber and polymer systems, both in the thermal and quenched cases.

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